Condensate Fluctuations in Trapped Bose Gases: Canonical vs. Microcanonical Ensemble *

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Abstract

We study the fluctuation of the number of particles in ideal Bose–Einstein condensates, both within the canonical and the microcanonical ensemble. Employing the Mellin–Barnes transformation, we derive simple expressions that link the canonical number of condensate particles, its fluctuation, and the difference between canonical and microcanonical fluctuations to the poles of a Zeta function that is determined by the excited single-particle levels of the trapping potential. For the particular examples of one- and three-dimensional harmonic traps we explore the microcanonical statistics in detail, with the help of the saddle-point method. Emphasizing the close connection between the partition theory of integer numbers and the statistical mechanics of ideal Bosons in one-dimensional harmonic traps, and utilizing thermodynamical arguments, we also derive an accurate formula for the fluctuation of the number of summands that occur when a large integer is partitioned.

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I. INTRODUCTION

The ideal Bose gas is customarily treated in the grand canonical ensemble, since the evaluation of the canonical partition sum is impeded by the constraint that the total particle number N be fixed. In contrast, after introducing a variable that is conjugate to N, the fugacity z, the computation of the ensuing grand canonical partition function $\Xi(z, \beta)$ requires merely the summation of geometric series, and all thermodynamic properties of the Bose gas are then obtained by taking suitable derivatives of $\Xi(z, \beta)$ with respect to z or the inverse temperature β.

There is, however, one serious failure of the grand canonical ensemble. Grand canonical statistics predicts that the mean-square fluctuation $\langle \delta^2 n_\nu \rangle_{gc}$ of the ν-th single-particle level's occupation equals $\langle n_\nu \rangle_{gc} (\langle n_\nu \rangle_{gc} + 1)$. Applied to the ground state $\nu = 0$, this gives

$$\langle \delta^2 n_0 \rangle_{gc} = \langle n_0 \rangle_{gc} (\langle n_0 \rangle_{gc} + 1)$$

even when the temperature T approaches zero, so that all N particles condense into the ground state. But the implication of huge fluctuations, $\langle \delta^2 n_0 \rangle_{gc} = N(N + 1)$, is clearly unacceptable; when all particles occupy the ground state, the fluctuation has to die out.

This grand canonical fluctuation catastrophe has been discussed by generations of physicists, and possible remedies have been suggested within the canonical framework [2–4]. After the recent realization of Bose–Einstein condensates of weakly interacting gases of alkali atoms [5–9] had brought the problem back into the focus of interest [10–13], significant steps towards its general solution could be made. Ideal condensate fluctuations have been computed for certain classes of single-particle spectra, i.e., for certain trap types, both within the canonical ensemble [11,14], where the gas is still exchanging energy with some hypothetical heat bath, and within the more appropriate microcanonical ensemble [10,15,16], where it is completely isolated. Interestingly, canonical and microcanonical fluctuations have been found to agree in the large-N-limit for one-dimensional harmonic trapping potentials [10,13], but to differ in the case of three-dimensional isotropic harmonic traps [11,15].

Yet, in the true spirit of theoretical physics one would clearly like to have more than merely some formulas for condensate fluctuations in particular traps. Can't one extract a common feature that underlies those formulas, such that simply inspecting that very feature allows one to determine, without any actual calculation, the temperature dependence of the condensate fluctuation, and to decide whether or not canonical and microcanonical fluctuations are asymptotically equal?

It is such a refined understanding that we aim at in the present work. As will be shown, the feature imagined above actually exists: It is the rightmost pole, in the complex t-plane, of the Zeta function

$$Z(\beta, t) \;=\; \sum_{\nu=1}^{\infty} \frac{1}{(\beta\varepsilon_\nu)^t}$$

that is furnished by the system's single-particle energies ε_ν. In order to substantiate this statement, we will proceed as follows: We start in the next section by deriving simple expressions that relate the canonical number of ground state particles $\langle n_0 \rangle_{cn}$, and its mean-square fluctuation $\langle \delta^2 n_0 \rangle_{cn}$, to $Z(\beta, t)$. The key point exploited there is the approximate equivalence of a trapped Bose gas in the condensate regime to a system of Boltzmannian harmonic oscillators. This equivalence, which holds irrespective of the particular form of the trapping potential, implies that both $\langle n_0 \rangle_{cn}$ and $\langle \delta^2 n_0 \rangle_{cn}$ can be expressed in terms of harmonic oscillator sums, which explain the emergence of the spectral Zeta function $Z(\beta, t)$ and can be computed with the help of well-established techniques [17]. In Section III we then evaluate these general canonical formulas for d-dimensional isotropic harmonic traps, where $Z(\beta, t)$ reduces to ordinary Riemann Zeta functions, and for anisotropic harmonic traps, where it leads to Zeta functions of the Barnes type.

In Section IV we compare the canonical statistics of harmonically trapped gases for $d = 1$ and $d = 3$ to their microcanonical counterparts. The strategy adopted there — the calculation of microcanonical moments from the easily accessible corresponding canonical moments by means of saddle-point inversions — is technically rather cumbersome and certainly not to be recommended if one merely wishes to obtain the microcanonical condensate fluctuations $\langle \delta^2 n_0 \rangle_{mc}$, but it explains in precise detail just how the difference between the canonical and the microcanonical ensemble comes into play, and why $\langle \delta^2 n_0 \rangle_{mc}$ becomes asymptotically equal to $\langle \delta^2 n_0 \rangle_{cn}$ in some cases, but not in others. A convenient expression for the immediate determination of $\langle \delta^2 n_0 \rangle_{cn} - \langle \delta^2 n_0 \rangle_{mc}$, based again on the spectral Zeta function $Z(\beta, t)$, is then derived in Section V. The final Section VI contains a concluding discussion; three appendices offer technical details.

Since we restrict ourselves to non-interacting Bose gases, the main value of the present work lies on the conceptual side — after all, the ideal Bose gas ought to be properly understood —, but it may well turn out to be of more than purely academical importance: After it has been demonstrated now that the s-wave scattering length in optically confined condensates can be tuned by varying an external magnetic field [18], the creation of almost ideal Bose–Einstein condensates might become feasible. If it did, then also the experimental investigation of the basic statistical questions studied here, such as the connection between the temperature dependence of the condensate fluctuation and the properties of the trap potential, should not remain out of reach.

Finally, there is still another appealing side-aspect: Since the microcanonical statistics of ideal Bosons in one-dimensional harmonic traps can be mapped to the partition theory of integer numbers, a natural by-product of our work is a fairly accurate formula for the fluctuation of the number of integer parts into which a large integer may by decomposed. The derivation of that formula in Section V is a beautiful example for the deep-rooted connection between partition theory and statistical mechanics, quite in the sense of Schrödinger's remark quoted above.

II. CANONICAL DESCRIPTION OF IDEAL BOSE–EINSTEIN CONDENSATES

We consider a gas of non-interacting Bose particles confined in a trap with discrete single-particle energies ε_ν ($\nu = 0, 1, 2, \ldots$) and stipulate that the ground state energy be equal to zero, $\varepsilon_0 = 0$. Starting from the grand canonical partition sum

$$\prod_{\nu=0}^{\infty} \frac{1}{1 - z \exp(-\beta \varepsilon_\nu)} \;=\; \Xi(z, \beta) \,, \tag{1}$$

where $\beta = 1/(k_B T)$ is the inverse temperature, we have the familiar expansion

$$\Xi(z, \beta) \;=\; \sum_{N=0}^{\infty} z^N \sum_E e^{-\beta E}\, \Omega(E|N) \,, \tag{2}$$

with coefficients $\Omega(E|N)$ denoting the number of microstates accessible to an N-particle gas with total excitation energy E. Combinatorically speaking, $\Omega(E|N)$ is the number of possibilities for sharing the energy E among *up to* N particles — the number N_{ex} of particles that are actually excited and thus carry a part of E remains unspecified.

The clear distinction between N and N_{ex} is the starting point for studying statistical properties of Bose–Einstein condensates in gases with fixed particle number. When N_{ex} out of N Bose particles are excited, there remain $N - N_{\mathrm{ex}}$ particles forming the condensate, and the corresponding number of microstates (that is, the number of possibilities for distributing the excitation energy E over *exactly* N_{ex} particles) is given by

$$\Omega(E|N_{\mathrm{ex}}) - \Omega(E|N_{\mathrm{ex}} - 1) \;\equiv\; \Phi(N_{\mathrm{ex}}|E) \,. \tag{3}$$

Within the *canonical* ensemble, i.e., if the N-particle gas is in contact with some heat bath of temperature T, the probability for finding N_{ex} excited particles can then be written as

$$p_{cn}(N_{\mathrm{ex}}, \beta) \;=\; \frac{\sum_E e^{-\beta E}\, \Phi(N_{\mathrm{ex}}|E)}{\sum_E e^{-\beta E} \sum_{N'_{\mathrm{ex}}=0}^{N} \Phi(N'_{\mathrm{ex}}|E)} \quad , \quad N_{\mathrm{ex}} \le N \,. \tag{4}$$

The expectation value $\langle N_{\mathrm{ex}} \rangle_{cn}$ with respect to this distribution yields the canonical ground state occupation number,

$$\langle n_0 \rangle_{cn} \;=\; N - \langle N_{\mathrm{ex}} \rangle_{cn} \,; \tag{5}$$

the canonical mean-square fluctuation of the number of condensate particles is identical to the fluctuation of the number of excited particles,

$$\begin{aligned}
\langle \delta^2 n_0 \rangle_{cn} &= \langle \delta^2 N_{\mathrm{ex}} \rangle_{cn} \\
&= \langle N_{\mathrm{ex}}^2 \rangle_{cn} - \langle N_{\mathrm{ex}} \rangle_{cn}^2 \,.
\end{aligned} \tag{6}$$

In order to calculate these cumulants, we consider the function

$$(1 - z)\, \Xi(z, \beta) \;\equiv\; \Xi_{\mathrm{ex}}(z, \beta) \,, \tag{7}$$

which satisfies the identities

$$\Xi_{\text{ex}}(z, \beta) = \sum_{N=0}^{\infty} \left(z^N - z^{N+1} \right) \sum_E e^{-\beta E} \, \Omega(E|N)$$

$$= \sum_{N=0}^{\infty} z^N \sum_E e^{-\beta E} \left[\Omega(E|N) - \Omega(E|N-1) \right] \tag{8}$$

with $\Omega(E|-1) = 0$. Hence, replacing the summation index N by N_{ex}, one finds

$$\Xi_{\text{ex}}(z, \beta) = \sum_{N_{\text{ex}}=0}^{\infty} z^{N_{\text{ex}}} \sum_E e^{-\beta E} \, \Phi(N_{\text{ex}}|E) \,. \tag{9}$$

On the other hand we have

$$\Xi_{\text{ex}}(z, \beta) = \prod_{\nu=1}^{\infty} \frac{1}{1 - z \exp(-\beta \varepsilon_\nu)} \,, \tag{10}$$

where, in contrast to Eq. (1), the product runs only over the excited states $\nu \geq 1$: *The grand canonical partition sum of a fictituous Bose gas which emerges from the actual gas by removing the single-particle ground state is the generating function for* $\Phi(N_{\text{ex}}|E)$. Differentiating this generating function k times, and then setting $z = 1$, one gets the canonical moments [1]

$$\left(z \frac{\partial}{\partial z} \right)^k \Xi_{\text{ex}}(z, \beta) \bigg|_{z=1} = \sum_E e^{-\beta E} \left(\sum_{N_{\text{ex}}=0}^{\infty} N_{\text{ex}}^k \, \Phi(N_{\text{ex}}|E) \right) \equiv M_k(\beta) \,. \tag{11}$$

In the customary grand canonical framework, z is identified with the fugacity and linked to the ground state occupation number $\langle n_0 \rangle_{gc}$ by $z = (1 + 1/\langle n_0 \rangle_{gc})^{-1}$. In that case z remains strictly less than unity, thus preventing the ground state factor in Eq. (1) from diverging. In contrast, z is no more than a formal parameter in the present analysis, entirely unrelated to the ground state occupation; and since the ground state factor is absent in the generating function $\Xi_{\text{ex}}(z, \beta)$, there is nothing to prevent us from fixing $z = 1$.

If the sum over N_{ex} in Eq. (11) did not range from 0 to ∞, but instead from 0 to the actual particle number N, as it does in the canonical distribution (4), then the ratio $M_1(\beta)/M_0(\beta)$ would be *exactly* equal to the canonical expectation value $\langle N_{\text{ex}} \rangle_{cn}$. But even if we do not have an exact equality here, the difference between these two quantities must be negligible *if there is a condensate*. This statement requires no proof, it is a mere tautology: a condensate can only be present if those microstates where the energy E is spread over all N particles are statistically negligible, so that also the microstates that would become available if additional zero-energy (ground state) particles were added to the gas cannot make themselves felt. Hence, in the presence of a Bose–Einstein condensate we have, for small k,

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[1]This corresponds to a trick suggested by D. H. Lehmer and taken up by L. B. Richmond for calculating k-th moments of partitions of integer numbers; see Ref. [19]. Note that the asymptotic moment formula derived in that paper is not correct for $k \geq 2$; the corrected formula is stated in Appendix C.

$$\sum_{N_{\text{ex}}=0}^{\infty} N_{\text{ex}}^k \, \Phi(N_{\text{ex}}|E) \;=\; \sum_{N_{\text{ex}}=0}^{N} N_{\text{ex}}^k \, \Phi(N_{\text{ex}}|E) \tag{12}$$

at least to a very good approximation, which gives both

$$\langle N_{\text{ex}} \rangle_{cn} \;=\; \frac{M_1(\beta)}{M_0(\beta)} \tag{13}$$

and

$$\langle \delta^2 N_{\text{ex}} \rangle_{cn} \;=\; \frac{M_2(\beta)}{M_0(\beta)} - \left(\frac{M_1(\beta)}{M_0(\beta)} \right)^2 . \tag{14}$$

The approximation (12), expressing the replacement of the actual condensate of $N - \langle N_{\text{ex}} \rangle_{cn}$ particles by a condensate consisting of infinitely many particles, can be interpreted in two different ways. On the one hand, the infinitely many ground state particles may be regarded as forming a particle reservoir for the excited-states subsystem. Such an approach to computing canonical condensate fluctuations had been suggested as early as 1956 by Fierz [2]; it corresponds to the "Maxwell's Demon Ensemble" recently put forward by Navez et al. [15].

The second interpretation rests on the observation that for $k = 0$ the approximation (12) takes the form

$$\sum_{N_{\text{ex}}=0}^{\infty} \Phi(N_{\text{ex}}|E) \;=\; \Omega(E|N) , \tag{15}$$

so that Eq. (11) gives

$$\sum_{E} e^{-\beta E} \, \Omega(E|N) \;=\; \prod_{\nu=1}^{\infty} \frac{1}{1 - \exp(-\beta \varepsilon_\nu)} \;\equiv\; Z(\beta) . \tag{16}$$

Since each factor $1/[1 - \exp(-\beta \varepsilon_\nu)]$ corresponds to a geometric series, i.e., to the canonical partition function of a simple harmonic oscillator with frequency $\varepsilon_\nu/\hbar$, Eq. (16) states that if there is a condensate, so that Eq. (15) holds, then the canonical partition function of an ideal Bose gas with arbitrary single-particle energies is well approximated by the canonical partition function of a system of distinguishable harmonic oscillators, each excited single-particle level ε_ν corresponding to an oscillator with frequency $\varepsilon_\nu/\hbar$. Thus, *for temperatures below the onset of Bose–Einstein condensation the thermodynamics of the actual Bose gas practically coincides with the thermodynamics of a Boltzmannian harmonic oscillator system*, regardless of the specific form of the trapping potential. For this reason, we will refer to the approximation (12) as the *oscillator approximation*. For the particular case of a three-dimensional isotropic harmonic trapping potential, the quality of this approximation has been confirmed in Ref. [20] by comparing the entropy of the actual Bose gas with that of its Boltzmannian substitute.

Within this oscillator approximation, the determination of the number $\langle N_{\text{ex}} \rangle_{cn}$ of excited particles, and of the canonical mean-square condensate fluctuation $\langle \delta^2 n_0 \rangle_{cn} = \langle \delta^2 N_{\text{ex}} \rangle_{cn}$, becomes remarkably simple. Doing the derivatives demanded by Eq. (11), we find

$$M_0(\beta) = Z(\beta) \tag{17}$$
$$M_1(\beta) = Z(\beta)S_1(\beta) \tag{18}$$
$$M_2(\beta) = Z(\beta)\left[S_1^2(\beta) + S_2(\beta)\right] , \tag{19}$$

with $Z(\beta)$ as given by Eq. (16), and

$$
\begin{aligned}
S_1(\beta) &= \sum_{\nu=1}^{\infty} \frac{1}{\exp(\beta\varepsilon_\nu) - 1} \\
&= \sum_{\nu=1}^{\infty} \sum_{r=0}^{\infty} \exp[-\beta\varepsilon_\nu(r+1)] ,
\end{aligned} \tag{20}
$$

$$
\begin{aligned}
S_2(\beta) &= \sum_{\nu=1}^{\infty} \frac{1}{\exp(\beta\varepsilon_\nu) - 1}\left(\frac{1}{\exp(\beta\varepsilon_\nu) - 1} + 1\right) \\
&= \sum_{\nu=1}^{\infty} \sum_{r=1}^{\infty} r \, \exp[-\beta\varepsilon_\nu r] .
\end{aligned} \tag{21}
$$

Computing the ratios $M_1(\beta)/M_0(\beta)$ and $M_2(\beta)/M_0(\beta)$ according to Eqs. (13) and (14), the oscillator partition function $Z(\beta)$ drops out (and, hence, does not even have to be evaluated here!), and we arrive at the appealing relations

$$\langle N_{\mathrm{ex}}\rangle_{cn} = S_1(\beta) \tag{22}$$
$$\langle \delta^2 N_{\mathrm{ex}}\rangle_{cn} = S_2(\beta) . \tag{23}$$

Since $1/[\exp(\beta\varepsilon_\nu) - 1] = \langle n_\nu\rangle_{gc}$ is just the grand canonical expectation value for the occupation of the ν-th excited state in a partially condensed Bose gas (the fugacity of which is $z = 1$), and $\langle n_\nu\rangle_{gc}\,(\langle n_\nu\rangle_{gc} + 1) = \langle \delta^2 n_\nu\rangle_{gc}$ is the corresponding grand canonical mean-square fluctuation, the respresentations (20) and (21) reveal that the canonical expectation value of the number of excited particles equals the grand canonical one, and that the canonical mean-square fluctuation of the ground state occupation number can simply be computed by adding the grand canonical fluctuations of the excited levels, subject to only the oscillator approximation. This is precisely what had been anticipated by Fierz [2], and what has also been exploited in a heuristic manner by Politzer [11] when investigating the three-dimensional harmonic trap.

For evaluating the sums $S_1(\beta)$ and $S_2(\beta)$ we employ the Mellin–Barnes integral representation [17]

$$e^{-\alpha} = \frac{1}{2\pi i} \int_{\tau - i\infty}^{\tau + i\infty} \mathrm{d}t \, \alpha^{-t}\, \Gamma(t) , \tag{24}$$

valid for real $\tau > 0$ and complex α with $\mathrm{Re}\,(\alpha) > 0$. This leads to

$$
\begin{aligned}
\langle N_{\mathrm{ex}}\rangle_{cn} &= \sum_{\nu=1}^{\infty} \sum_{r=0}^{\infty} \frac{1}{2\pi i} \int_{\tau - i\infty}^{\tau + i\infty} \mathrm{d}t \, \frac{\Gamma(t)}{[\beta\varepsilon_\nu(r+1)]^t} \\
&= \frac{1}{2\pi i} \int_{\tau - i\infty}^{\tau + i\infty} \mathrm{d}t \sum_{\nu=1}^{\infty} \sum_{r=0}^{\infty} \frac{\Gamma(t)}{[\beta\varepsilon_\nu(r+1)]^t} \\
&= \frac{1}{2\pi i} \int_{\tau - i\infty}^{\tau + i\infty} \mathrm{d}t \, \Gamma(t) Z(\beta, t)\zeta(t) ,
\end{aligned} \tag{25}
$$

where $\zeta(t) = \sum_{r=1}^{\infty} r^{-t}$ denotes the Riemann Zeta function, and we have introduced the spectral Zeta function

$$Z(\beta, t) = \sum_{\nu=1}^{\infty} \frac{1}{(\beta \varepsilon_\nu)^t} \tag{26}$$

that embodies the necessary information about the trap spectrum. In the same way we find the remarkably similar-looking equation

$$\langle \delta^2 N_{\text{ex}} \rangle_{cn} = \frac{1}{2\pi i} \int_{\tau - i\infty}^{\tau + i\infty} dt\, \Gamma(t) Z(\beta, t) \zeta(t - 1) \; . \tag{27}$$

It should be noted that interchanging summations and integration in Eq. (25), and in the analogous derivation of the canonical fluctuation formula (27), requires the absolute convergence of the emerging sums. Therefore, the real number τ has to be chosen such that the path of integration up the complex t-plane lies to the right of the poles of both Zeta functions.

Now the temperature dependence of $\langle N_{\text{ex}} \rangle_{cn}$ or $\langle \delta^2 N_{\text{ex}} \rangle_{cn}$ is determined by the pole of the integrand (25) or (27) that lies farthest to the right. Since $\Gamma(t)$ has poles merely at $t = 0, -1, -2, \ldots$, the decisive pole is provided *either* by the Riemann Zeta function $\zeta(t)$ or $\zeta(t - 1)$, respectively, *or* by its spectral opponent $Z(\beta, t)$, which depends on the particular trap under study [16]. This competition will be discussed in detail in the following section, focussing on harmonic trapping potentials.

III. ISOTROPIC AND ANISOTROPIC HARMONIC TRAPS

The evaluation of the canonical relations (25) and (27) reduces to a mere formality if the pole structure of the spectral Zeta function (26) is known. The simplest examples are provided by d-dimensional isotropic harmonic traps, since then $Z(\beta, t)$ becomes a sum of Riemannian Zeta functions. Namely, denoting the angular frequency of such a trap by ω, the degree of degeneracy g_ν of a single-particle state with excitation energy $\nu \hbar \omega$ is

$$g_\nu = \binom{\nu + d - 1}{d - 1} \; , \tag{28}$$

so that $Z(\beta, t)$ acquires the form

$$Z(\beta, t) = (\beta \hbar \omega)^{-t} \sum_{\nu=1}^{\infty} \frac{g_\nu}{\nu^t} \; , \tag{29}$$

giving in explicit terms

$$\begin{aligned}
Z(\beta, t) &= (\beta \hbar \omega)^{-t} \zeta(t) & \text{for } d = 1 \; , \\
Z(\beta, t) &= (\beta \hbar \omega)^{-t} \left[\zeta(t - 1) + \zeta(t) \right] & \text{for } d = 2 \; , \\
Z(\beta, t) &= (\beta \hbar \omega)^{-t} \left[\zeta(t - 2)/2 + 3\zeta(t - 1)/2 + \zeta(t) \right] & \text{for } d = 3 \; .
\end{aligned} \tag{30}$$

We now aim at the temperature dependence of $\langle N_{\text{ex}} \rangle_{cn}$ and $\langle \delta^2 N_{\text{ex}} \rangle_{cn}$ for temperatures below the onset of a "macroscopic" ground state occupation, so that the oscillator approximation

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retains its validity, but well above the level spacing temperature $\hbar\omega/k_B$, so that $\beta\hbar\omega \ll 1$. Such a temperature interval exists if the particle number N is sufficiently large, since the condensation temperature generally increases with N. The desired asymptotic T-dependence can then directly be read off from the residue of the rightmost pole of the respective integrand (25) or (27). Since $\zeta(z)$ has merely a single pole at $z = 1$, simple and with residue $+1$, namely [21]

$$\zeta(z) \approx \frac{1}{z-1} + \gamma \tag{31}$$

for z close to 1, the calculation of that residue is particularly easy if the rightmost pole in (25) or (27) is simple. In the case of a double pole we also need the identity

$$\Gamma'(n) = \Gamma(n)\,\psi(n)$$
$$= \Gamma(n)\left(-\gamma + \sum_{m=1}^{n-1}\frac{1}{m}\right) \tag{32}$$

for the Psi function at integer arguments, with $\gamma \approx 0.5772$ denoting Euler's constant. This is the only technical knowledge required for computing the number of excited particles, and its fluctuation, in a d-dimensional isotropic harmonic trap within the canonical ensemble:

(i) For $d = 1$, the number of excited particles is governed by the double pole at $t = 1$ which emerges since $Z(\beta, t)$ now is proportional to $\zeta(t)$, whereas the mean-square fluctuation is dominated by the simple pole of $\zeta(t-1)$ at $t = 2$:

$$\langle N_{\text{ex}}\rangle_{cn} = \frac{k_B T}{\hbar\omega}\left[\ln\left(\frac{k_B T}{\hbar\omega}\right) + \gamma\right] \tag{33}$$

$$\langle \delta^2 N_{\text{ex}}\rangle_{cn} = \left(\frac{k_B T}{\hbar\omega}\right)^2 \zeta(2)\,. \tag{34}$$

(ii) For $d = 2$, the rightmost pole of $Z(\beta, t)$ has moved to $t = 2$ and thus determines $\langle N_{\text{ex}}\rangle_{cn}$ all by itself, but now the product $Z(\beta, t)\zeta(t-1)$ provides a double pole that governs the asymptotics of the fluctuation:

$$\langle N_{\text{ex}}\rangle_{cn} = \left(\frac{k_B T}{\hbar\omega}\right)^2 \zeta(2) \tag{35}$$

$$\langle \delta^2 N_{\text{ex}}\rangle_{cn} = \left(\frac{k_B T}{\hbar\omega}\right)^2 \left[\ln\left(\frac{k_B T}{\hbar\omega}\right) + \gamma + 1 + \zeta(2)\right]\,. \tag{36}$$

(iii) For $d = 3$, the pole of the spectral Zeta function $Z(\beta, t)$ at $t = 3$ wins in both cases:

$$\langle N_{\text{ex}}\rangle_{cn} = \left(\frac{k_B T}{\hbar\omega}\right)^3 \zeta(3) \tag{37}$$

$$\langle \delta^2 N_{\text{ex}}\rangle_{cn} = \left(\frac{k_B T}{\hbar\omega}\right)^3 \zeta(2)\,. \tag{38}$$

Of course, these results remain valid only as long as $\langle N_{\text{ex}} \rangle_{cn} < N$. Equating $\langle N_{\text{ex}} \rangle_{cn}$ and N for $d = 3$, e.g., one finds the large-N condensation temperature

$$T_0 = \frac{\hbar\omega}{k_B} \left(\frac{N}{\zeta(3)} \right)^{1/3} \tag{39}$$

for an ideal gas in a three-dimensional harmonic trap that exchanges energy, but no particles, with a heat bath. As expected, this result agrees with the one provided by the familiar grand canonical ensemble [22]. Even more, taking into account also the next-to-leading pole, one obtains the improvement

$$\langle N_{\text{ex}} \rangle_{cn} = \zeta(3) \left(\frac{k_B T}{\hbar\omega} \right)^3 + \frac{3}{2} \zeta(2) \left(\frac{k_B T}{\hbar\omega} \right)^2 \tag{40}$$

to Eq. (37), implying that for Bose gases with merely a moderate number of particles the actual condensation temperature T_C is lowered by terms of the order $N^{-1/3}$ against T_0,

$$T_C = T_0 \left[1 - \frac{\zeta(2)}{2\,\zeta(3)^{2/3}} \frac{1}{N^{1/3}} \right] . \tag{41}$$

Even this improved canonical expression equals its grand canonical counterpart [23–26].

These examples nicely illustrate the working principle of the basic integral representations (25) and (27): There are two opponents that place poles on the positive real axis, namely the spectral Zeta function $Z(\beta, t)$ on the one hand, which depends on the particular trap, and $\zeta(t)$ or $\zeta(t-1)$ on the other, which are entirely independent of the system. For both the number of excited particles and its mean-square fluctuation, the exponent of T is given by the location of the pole farthest to the right. Whereas the pole of $\zeta(t)$ and $\zeta(t-1)$ does, naturally, not depend on the spatial dimension d, the asymptotically relevant pole of $Z(\beta, t)$ lies at $t = d$ and thus moves with increasing d to the right, governing $\langle N_{\text{ex}} \rangle_{cn}$ above $d = 1$ and $\langle \delta^2 N_{\text{ex}} \rangle_{cn}$ above $d = 2$.

But what about the *anisotropic* traps that play a major role in present experiments? With the ground state energy set to zero, and angular trap frequencies ω_i ($i = 1, \ldots, d$), the energy levels then are

$$\varepsilon_{\nu_1, \ldots, \nu_d} = \hbar(\omega_1 \nu_1 + \ldots + \omega_d \nu_d) \equiv \hbar\vec{\omega}\vec{\nu} , \qquad \vec{\nu} \in \mathbb{N}_0^d . \tag{42}$$

The spectral Zeta function

$$Z(\beta, t) = \sum_{\vec{\nu} \in \mathbb{N}_0^d / \{0\}} \frac{1}{(\beta\hbar\vec{\omega}\vec{\nu})^t} \tag{43}$$

now is a Zeta function of the Barnes type [27] (see also Ref. [28]). Its rightmost pole is located at $t = d$, with residue

$$\text{res}\, Z(\beta, d) = \frac{1}{\Gamma(d)} \left(\frac{k_B T}{\hbar\Omega} \right)^d , \tag{44}$$

where we have introduced the geometric mean Ω of the trap frequencies,

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$$\Omega = \left(\prod_{i=1}^{d} \omega_i \right)^{1/d} \tag{45}$$

The derivation of Eq. (44) is sketched in Appendix A.

The asymptotic evaluation of the canonical formulas (25) and (27) now requires $\beta \hbar \omega_i \ll 1$ for all i. If this condition is not met, since, for instance, one of the trapping frequencies is much larger than the others, one has to treat the entailing dimensional crossover effects [29] by keeping the corresponding part of $Z(\beta, t)$ as a discrete sum. In the following we will assume merely moderate anisotropy, so that the above inequalities are satisfied.

For two-dimensional anisotropic harmonic traps, the computation of the canonically expected number of excited particles, and its fluctuation, then leads to

$$\langle N_{\text{ex}} \rangle_{cn} = \left(\frac{k_B T}{\hbar \Omega} \right)^2 \zeta(2) \tag{46}$$

$$\langle \delta^2 N_{\text{ex}} \rangle_{cn} = \left(\frac{k_B T}{\hbar \Omega} \right)^2 \left[\ln \left(\frac{k_B T}{\hbar (\omega_1 + \omega_2)} \right) + \left(\frac{\omega_1}{\omega_2} + \frac{\omega_2}{\omega_1} \right) \zeta(2) + I(\omega_1, \omega_2) \right] , \tag{47}$$

with

$$I(\omega_1, \omega_2) = \int_0^\infty d\alpha \, \alpha e^{-\left(\sqrt{\frac{\omega_1}{\omega_2}} + \sqrt{\frac{\omega_2}{\omega_1}} \right) \alpha} \left(\frac{1}{\left(1 - e^{-\sqrt{\frac{\omega_1}{\omega_2}} \alpha} \right) \left(1 - e^{-\sqrt{\frac{\omega_2}{\omega_1}} \alpha} \right)} - \frac{1}{\alpha^2} \right) . \tag{48}$$

Equation (47) reveals a rather complicated dependence of the fluctuation $\langle \delta^2 N_{\text{ex}} \rangle_{cn}$ on the trap frequencies ω_1 and ω_2. The comparatively simple form of the previous Eq. (36) for an isotropic trap has its technical reason in the simple expansion (31) of $\zeta(z)$ around its pole. In contrast, for two-dimensional anisotropic traps we need the analogous expansion of the Barnes Zeta function (43) for $d = 2$. The finite part of this expansion, corresponding to Euler's constant γ in Eq. (31), now becomes a function of the frequencies ω_1 and ω_2 that enters into the above result. Details are explained in Appendix B, where we also show the identity

$$I(\omega, \omega) = \gamma + 1 + \ln 2 - \zeta(2) , \tag{49}$$

which ensures that Eq. (47) reduces to the isotropic result (36) for $\omega_1 = \omega_2 = \omega$.

For any dimension $d \geq 3$, it is the pole of $Z(\beta, t)$ at $t = d$ which determines the behaviour of both $\langle N_{\text{ex}} \rangle_{cn}$ and $\langle \delta^2 N_{\text{ex}} \rangle_{cn}$:

$$\langle N_{\text{ex}} \rangle_{cn} = \left(\frac{k_B T}{\hbar \Omega} \right)^d \zeta(d) \tag{50}$$

$$\langle \delta^2 N_{\text{ex}} \rangle_{cn} = \left(\frac{k_B T}{\hbar \Omega} \right)^d \zeta(d - 1) . \tag{51}$$

The difference between the isotropic and the mildly anisotropic case now merely consists in the replacement of the frequency ω by the geometric mean Ω.

IV. A SADDLE-POINT APPROACH TO MICROCANONICAL STATISTICS

When the ideal N-particle Bose gas is completely isolated from its surrounding, carrying a total excitation energy E, one has to resort to the microcanonical framework. The microcanonical counterpart of the distribution (4), that is, the probability for finding N_{ex} out of the N isolated particles in an excited state, is given by

$$p_{mc}(N_{\mathrm{ex}}, E) \;=\; \frac{\Phi(N_{\mathrm{ex}}|E)}{\sum_{N_{\mathrm{ex}}'=0}^{N} \Phi(N_{\mathrm{ex}}'|E)} \quad , \quad N_{\mathrm{ex}} \le N \; . \tag{52}$$

It is quite instructive to copy the previous canonical analysis as far as possible, in order to pin down precisely how the difference between the canonical and the microcanonical ensemble manifests itself. Hence, we wish to calculate the k-th moments

$$\mu_k(E) \;=\; \sum_{N_{\mathrm{ex}}=0}^{N} N_{\mathrm{ex}}^k \, \Phi(N_{\mathrm{ex}}|E) \tag{53}$$

of this distribution (52), which yield the microcanonical expectation value

$$\langle N_{\mathrm{ex}} \rangle_{mc} \;=\; \frac{\mu_1(E)}{\mu_0(E)} \tag{54}$$

of the number of excited particles, and the corresponding mean-square fluctuation

$$\langle \delta^2 N_{\mathrm{ex}} \rangle_{mc} \;=\; \frac{\mu_2(E)}{\mu_0(E)} - \left(\frac{\mu_1(E)}{\mu_0(E)} \right)^2 \; . \tag{55}$$

Provided the energy E is so low that a major fraction of the particles remains in the ground state, i.e., if $\langle N_{\mathrm{ex}} \rangle_{mc}$ is sufficiently small as compared to N, we can again employ the oscillator approximation (12), and compute the microcanonical moments $\mu_k(E)$ from the easily accessible canonical moments (11) by means of saddle-point inversions.

To see in detail how this works, let us first carry through this program for the paradigmatic example of an isolated ideal Bose gas trapped by a one-dimensional harmonic oscillator potential. For ease of notation, we introduce the dimensionless variables $a = \beta\hbar\omega$, characterizing the inverse temperature, and $n = E/(\hbar\omega)$, corresponding to the total number of excitation quanta. We are thus working in the regime $a \ll 1$, $n \gg 1$. Again, this is compatible with the presence of a condensate if the particle number N is large. Writing $\mu_k(n)$, $Z(a)$, $S_1(a)$, and $S_2(a)$ instead of $\mu_k(E)$, $Z(\beta)$, $S_1(\beta)$, and $S_2(\beta)$ (see Eqs. (17) – (19)), and defining

$$H_0(a) \equiv 1 \tag{56}$$
$$H_1(a) \equiv S_1(a) \tag{57}$$
$$H_2(a) \equiv S_1^2(a) + S_2(a) \; , \tag{58}$$

the inversion formula acquires the form [30]

$$\mu_k(n) \;=\; \left. \frac{e^{na} \, Z(a) \, H_k(a)}{\left(-2\pi \frac{\partial n}{\partial a} \right)^{1/2}} \right|_{a=a_k(n)} \tag{59}$$

for $k = 0$, 1, and 2. It is crucial to note that each moment requires its own saddle-point parameter $a_k(n)$, obtained by inverting the corresponding saddle-point equation

$$n = -\frac{\mathrm{d}}{\mathrm{d}a}\ln Z(a) - \frac{\mathrm{d}}{\mathrm{d}a}\ln H_k(a) . \tag{60}$$

In contrast to the canonical case, we now need to evaluate the partition sum

$$Z(a) = \prod_{\nu=1}^{\infty} \frac{1}{1 - \exp(-a\nu)} \tag{61}$$

for $a \ll 1$. This partition sum actually is a well-studied object in the theory of modular functions; it satisfies a fairly interesting functional equation that allows one to extract the desired small-a-behaviour straight away [31,32]. In view of the intended transfer of the method to other trap types, we refrain from using this particular functional equation here, and resort once more to the Mellin–Barnes techniques. In this way we get

$$\begin{aligned}
\ln Z(a) &= -\sum_{\nu=1}^{\infty} \ln(1 - e^{-a\nu}) \\
&= \frac{1}{2\pi i} \int_{\tau-i\infty}^{\tau+i\infty} \mathrm{d}t \, a^{-t}\Gamma(t)\zeta(t)\zeta(t+1) ,
\end{aligned} \tag{62}$$

so that the dominant pole at $t = 1$ gives the approximation $\ln Z(a) \approx \zeta(2)/a$. However, in order to derive a proper asymptotic formula for $Z(a)$ we have to expand $\ln Z(a)$ up to terms of the order $O(a^0)$ inclusively, which necessitates to take into account also the double pole of the integrand (62) that lies at $t = 0$. Since the residue of this pole reads

$$-\zeta(0)\ln a + \zeta'(0) = \frac{1}{2}\ln a - \frac{1}{2}\ln 2\pi , \tag{63}$$

we obtain the desired approximation

$$\ln Z(a) = \frac{\zeta(2)}{a} + \frac{1}{2}\ln\frac{a}{2\pi} + O(a) . \tag{64}$$

With $H_1(a)$ and $H_2(a)$ as determined by Eqs. (33) and (34), the equations (60) for the saddle-point parameters then adopt the form

$$n = \frac{\zeta(2)}{a^2} + \frac{c(k)}{a} , \tag{65}$$

where

$$\begin{aligned}
c(0) &= -1/2 \\
c(1) &= -1/2 + 1 \\
c(2) &= -1/2 + 2 .
\end{aligned} \tag{66}$$

Inverting up to the required order $O(n^0)$, one finds

$$\frac{1}{a_k(n)} = \frac{\sqrt{6n}}{\pi} - \frac{3\,c(k)}{\pi^2} , \tag{67}$$

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hence

$$na_k(n) + \ln Z(a_k(n)) = \pi\sqrt{\frac{2n}{3}} + \frac{1}{2}\ln\left(\frac{1}{2\sqrt{6n}}\right) . \tag{68}$$

The important point to observe here is that the moment-dependent number $c(k)$ *drops out*, so that the factors $e^{n\,a_k(n)} Z(a_k(n))$ entering the inversion formula (59) become asymptotically equal for all k. Moreover, also the saddle-point corrections

$$\left(-2\pi\frac{\partial n}{\partial a}\right)^{-1/2}\Bigg|_{a=a_k(n)} = \sqrt{\frac{3}{2}}\,(6n)^{-3/4} \tag{69}$$

do not develop a significant k-dependence, so that these parts cancel when forming the ratio (54). Hence, we arrive at

$$\frac{\mu_1(n)}{\mu_0(n)} = H_1(a_1(n)) = S_1(a_1(n)) , \tag{70}$$

indicating that the microcanonical expectation value for the number of excited particles becomes equal to the canonical expression (22) in the asymptotic regime, where the difference between the saddle-point parameter $a_1(n)$ and the true inverse temperature $a_0(n)$ is negligible. Utilizing the asymptotic temperature–energy relation $k_B T/(\hbar\omega) = \sqrt{6n}/\pi$ obtained from Eq. (67), the microcanonical counterpart to Eq. (33) reads

$$\langle N_{\text{ex}}\rangle_{mc} = \frac{\sqrt{6n}}{\pi}\left[\ln\left(\frac{\sqrt{6n}}{\pi}\right) + \gamma\right] . \tag{71}$$

The calculation of the microcanonical condensate fluctuations requires more care. The canonical expression (23) had been an immediate consequence of the definition (14) and Eqs. (17) – (19), relying on the cancellation $[S_1^2(\beta) + S_2(\beta)] - S_1^2(\beta) = S_2(\beta)$, but now two different saddle-point parameters enter into the corresponding difference

$$H_2(a_2(n)) - H_1^2(a_1(n)) = S_2(a_2(n)) + \left(S_1^2(a_2(n)) - S_1^2(a_1(n))\right) , \tag{72}$$

indicating that the microcanonical fluctuation might deviate from the canonical one. However, for the one-dimensional oscillator trap we find that $S_1^2(a_2(n)) - S_1^2(a_1(n))$ is merely of the order $O(\sqrt{n}\ln^2 n)$, and thus asymptotically negligible in comparison to $S_2(a_2(n)) = n$. Therefore, for large n we have

$$\frac{\mu_2(n)}{\mu_0(n)} - \left(\frac{\mu_1(n)}{\mu_0(n)}\right)^2 = S_2(a_2(n)) , \tag{73}$$

meaning

$$\langle\delta^2 N_{\text{ex}}\rangle_{mc} = n , \tag{74}$$

so that the microcanonical fluctuation of the number of excited Bose particles in a one-dimensional harmonic trap, considered for energies such that on the average a fraction of

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the particles stays in the ground state, *coincides* asymptotically with the canonical fluctuation (34).

This analysis can directly be translated into the language of the theory of partitions of integer numbers [33]. Distributing n excitation quanta among ideal Bose particles, stored in a one-dimensional harmonic trap, is tantamount to partitioning the number n into summands; a particle occupying the ν-th excited oscillator state gives a summand of magnitude ν. In fact, utilizing Eqs. (68) and (69) for computing $\mu_0(n)$ according to Eq. (59), one finds

$$\mu_0(n) \; = \; \frac{1}{4\sqrt{3}n} \exp\left(\pi\sqrt{\frac{2n}{3}}\right) \; , \tag{75}$$

which is just the celebrated Hardy–Ramanujan formula for the total number of *unrestricted* partitions of n [31], corresponding to the number of microstates that are accessible to the Bose particles when their common excitation energy is $n\hbar\omega$, provided that n does not exceed the particle number N. For higher energies, the number of microstates equals the number of partitions that are *restricted* by the requirement that there be no more than N summands, since the n quanta cannot be distributed over more than the N available particles. However, as long as the distribution (52) remains sharply peaked around some value $\widehat{N}_{\mathrm{ex}} \approx \langle N_{\mathrm{ex}} \rangle_{mc} < N$, even though n may be substantially larger than N, the difference between the number of these restricted and that of the unrestricted partitions is insignificant, and neglecting this difference is nothing but the oscillator approximation (12) for $k = 0$.

From the viewpoint of partition theory, Eq. (71) gives the expected number of summands in a partition of n — randomly partitioning $n = 1000$, for instance, one expects roughly 93 summands — and Eq. (74) contains the remarkable statement that the r.m.s.-fluctuation of the number of parts into which n can be decomposed becomes just $\sqrt{n}$ in the asymptotic limit [16]. Higher cumulants $\kappa_m(n)$ of the distribution which describes the number of summands in unrestricted partitions of n can be obtained by following the same strategy as outlined above for calculating $\kappa_2(n) = n$, leading to, e.g.,

$$\kappa_3(n) \; = \; \frac{12\sqrt{6}\,\zeta(3)}{\pi^3}\, n^{3/2} \tag{76}$$

and

$$\kappa_4(n) \; = \; \frac{12}{5}\, n^2 \; . \tag{77}$$

This indicates deviations from a Gaussian distribution, for which all cumulants higher than the second are zero. A general asymptotic formula for the partition moments $\mu_k(n)$ for arbitrary k, together with a check of this formula against exact data for $k = 0, \ldots, 3$, can be found in Appendix C.

It is conceptually important to know that the fluctuation formula (74) for the harmonically trapped one-dimensional Bose gas can also be obtained *without* invoking the oscillator approximation, since the number of restricted partitions, and hence the entire distribution (52), can be well approximated with the help of an asymptotic expression due to Erdös and Lehner [34,10]. However, that approach depends on a specific asymptotic result that applies to the one-dimensional harmonic trap only, whereas the present method is capable of some generalization.

The preceding microcanonical analysis of the ideal Bose–Einstein condensate in a one-dimensional oscillator trap might appear like much ado about nothing: we have been careful to keep track of three slightly different saddle-point parameters, but in the end this distinction turned out to be insignificant, and we have merely recovered the canonical results. But this is not true in general; the following reasoning will show that (and why) a condensate in a three-dimensional isotropic harmonic trapping potential behaves differently. In this case we again face a partition-type problem, since the total excitation energy E remains an integer multiple of a basic quantum $\hbar\omega$. We can then virtually retrace the steps that have led for $d = 1$ to the microcanonical formulas (71) and (74): Starting from the partition sum

$$Z(a) = \prod_{\nu=1}^{\infty} \frac{1}{[1 - \exp(-a\nu)]^{(\nu+1)(\nu+2)/2}} \tag{78}$$

and applying the Mellin–Barnes transformation, one readily finds [2]

$$\ln Z(a) = \frac{\zeta(4)}{a^3} + \frac{3}{2}\frac{\zeta(3)}{a^2} + \frac{\zeta(2)}{a} + \frac{5}{8}\ln a$$
$$- \frac{1}{2}\ln 2\pi + \frac{3}{2}\zeta'(-1) + \frac{1}{2}\zeta'(-2) + O(a) , \tag{79}$$

which, together with the canonical expressions (37) and (38) that now define $H_1(a)$ and $H_2(a)$ via Eqs. (57) and (58), yields the saddle-point equations

$$n = \frac{3\zeta(4)}{a^4} + \frac{3\zeta(3)}{a^3} + \frac{\zeta(2)}{a^2} + \frac{c(k)}{a} \tag{80}$$

with

$$c(0) = -5/8$$
$$c(1) = -5/8 + 3$$
$$c(2) = -5/8 + 6 . \tag{81}$$

Again, these equations differ only to the order $O(a^{-1})$, and again the moment-dependent coefficient $c(k)$ drops out when computing $e^{n\, a_k(n)}Z(a_k(n))$ up to the asymptotically relevant terms of order $O(n^0)$:

$$na_k(n) + \ln Z(a_k(n)) = 4\zeta(4)\left(\frac{n}{3\zeta(4)}\right)^{3/4} + \frac{3}{2}\zeta(3)\left(\frac{n}{3\zeta(4)}\right)^{1/2}$$
$$+ \left[\zeta(2) - \frac{3}{8}\frac{\zeta(3)^2}{\zeta(4)}\right]\left(\frac{n}{3\zeta(4)}\right)^{1/4} - \frac{5}{32}\ln\left(\frac{n}{3\zeta(4)}\right)$$
$$+ \frac{\zeta(3)^3}{8\,\zeta(4)^2} - \frac{\zeta(2)\zeta(3)}{4\,\zeta(4)} - \frac{1}{2}\ln 2\pi + \frac{3}{2}\zeta'(-1) + \frac{1}{2}\zeta'(-2) . \tag{82}$$

---

[2]This expansion had already been derived in 1951 by V.S. Nanda with the help of the Euler–Maclaurin summation formula, see Ref. [35]. The Mellin–Barnes approach followed in the present work is *much* simpler, since it provides immediate access to the analytically continued Riemann Zeta function.

It is clear that this cancellation is quite general. Namely, for a d-dimensional isotropic harmonic trapping potential one has

$$\ln Z(a) = \frac{\zeta(d+1)}{a^d} + \dots \, , \tag{83}$$

and the saddle-point equations become

$$n = \frac{d\,\zeta(d+1)}{a^{d+1}} + \dots + \frac{c(k)}{a} \, , \tag{84}$$

hence

$$\frac{1}{a_k(n)} = \left(\frac{n}{d\,\zeta(d+1)} \right)^{1/(d+1)} + \dots - \frac{c(k)}{d(d+1)\,\zeta(d+1)} \left(\frac{n}{d\,\zeta(d+1)} \right)^{-(d-1)/(d+1)} . \tag{85}$$

When computing $na_k(n) + \ln Z(a_k(n))$, the product $na_k(n)$ contributes a term $c(k)$ that originates from the $O(a^{-1})$-term in Eq. (84). Otherwise, relevant k-dependent contributions enter into $na_k(n) + \ln Z(a_k(n))$ only via the leading terms of order $O(a^{-d})$ that stem from Eq. (83) on the one hand, and Eq. (84) multiplied by a on the other, summing up to

$$(d+1)\,\zeta(d+1) \times \left[d \left(\frac{n}{d\,\zeta(d+1)} \right)^{(d-1)/(d+1)} \right]$$

$$\times \left[\frac{-c(k)}{d(d+1)\,\zeta(d+1)} \left(\frac{n}{d\,\zeta(d+1)} \right)^{-(d-1)/(d+1)} \right] = -c(k) \tag{86}$$

and thus annihilating $c(k)$.

This little calculation, together with the inversion formula (59), shows explicitly that the microcanonical expectation values $\langle N_{\mathrm{ex}} \rangle_{mc}$ for d-dimensional isotropic harmonic traps become asymptotically equal to their canonical counterparts: Forming the ratio (54), the factors $e^{na} Z(a)(-2\pi \partial n/\partial a)^{-1/2}$ cancel even when evaluated at the slightly different saddle-point parameters $a_1(n)$ and $a_0(n)$, so that we are left with

$$\langle N_{\mathrm{ex}} \rangle_{mc} = S_1(a_1(n)) \, . \tag{87}$$

The asymptotic equality of $\langle N_{\mathrm{ex}} \rangle_{mc}$ and $\langle N_{\mathrm{ex}} \rangle_{cn}$ then follows by observing that $a_1(n)$ becomes asymptotically equal to the true inverse temperature $a_0(n)$.

The computation of the microcanonical condensate fluctuation along these lines, however, is a much more delicate matter. Returning to the particular example $d = 3$ for the sake of definiteness, both canonical expectation values $\langle N_{\mathrm{ex}} \rangle_{cn} = S_1(a)$ and $\langle \delta^2 N_{\mathrm{ex}} \rangle_{cn} = S_2(a)$ are determined by the *same* simple pole of $Z(\beta, t)$ at $t = 3$, which means that both $S_1(a)$ and $S_2(a)$ are proportional to a^{-3}. This, in turn, implies that in contrast to the one-dimensional case the difference $S_1^2(a_2(n)) - S_1^2(a_1(n))$ appearing in Eq. (72) now is of the *same* order as $S_2(a_2(n))$ itself, so that here the quite innocent-looking difference between the saddle-point equations (80), even though only of the order $O(a^{-1})$ and apparently hidden behind terms of order $O(a^{-4})$ — thus being overwhelmed much stronger than for $d = 1$ — *must* lead to an asymptotic difference between canonical and microcanonical condensate fluctuations: The

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exponent of T will be the same, but the prefactors will differ. This observation forces us to evaluate Eq. (55) very carefully. We may not simply rely on the cancellation of $c(k)$ as found in Eq. (82), but have to expand both ratios $\mu_2(n)/\mu_0(n)$ and $\mu_1(n)/\mu_0(n)$ consistently up to terms of order $O(a_k(n)^{-3}) = O(n^{3/4})$. This forces us to expand $na_k(n) + \ln Z(a_k(n))$, as well as the saddle-point corrections, even up to terms of the order $O(n^{-3/4})$! Detailed analysis shows that such an expansion is possible even with only the saddle-point equations (80) as input, although this is not immediately obvious. Proceeding in this manner, we find

$$
\begin{aligned}
\langle \delta^2 N_{\mathrm{ex}} \rangle_{mc} &= \left[1 + \frac{33}{12\,\zeta(4)} \left(\frac{3\zeta(4)}{n} \right)^{3/4} \right] H_2(a_2(n)) - \left[1 + \frac{2}{\zeta(4)} \left(\frac{3\zeta(4)}{n} \right)^{3/4} \right] H_1^2(a_1(n)) \\
&= S_2(a_2(n)) + \left(S_1^2(a_2(n)) - S_1^2(a_1(n)) \right) + \frac{3}{4} \frac{\zeta(3)^2}{\zeta(4)} \left(\frac{n}{3\zeta(4)} \right)^{3/4} .
\end{aligned}
\tag{88}
$$

The $O(n^{-3/4})$-corrections in the square brackets arise because the inverse temperature $a_0(n)$ differs from the saddle-point parameters $a_2(n)$ and $a_1(n)$; this is what causes the last term in the second equation. Since, moreover,

$$
S_1^2(a_2(n)) - S_1^2(a_1(n)) = -\frac{3}{2} \frac{\zeta(3)^2}{\zeta(4)} \left(\frac{n}{3\zeta(4)} \right)^{3/4} ,
\tag{89}
$$

we finally arrive at

$$
\begin{aligned}
\langle \delta^2 N_{\mathrm{ex}} \rangle_{mc} &= \left[\zeta(2) - \frac{3}{4} \frac{\zeta(3)^2}{\zeta(4)} \right] \left(\frac{n}{3\zeta(4)} \right)^{3/4} \\
&= \left[\zeta(2) - \frac{3}{4} \frac{\zeta(3)^2}{\zeta(4)} \right] \left(\frac{k_B T}{\hbar\omega} \right)^3 .
\end{aligned}
\tag{90}
$$

This quantifies what we have anticipated: Apparently tiny differences between the three saddle-point parameters conspire to lower the microcanonical mean-square condensate fluctuation against the canonical result (38), as a consequence of the fact that the rightmost pole of $Z(\beta, t)$ governs both $\langle N_{\mathrm{ex}} \rangle_{cn} = S_1(\beta)$ and $\langle \delta^2 N_{\mathrm{ex}} \rangle_{cn} = S_2(\beta)$. For the one-dimensional harmonic trap, where $\langle N_{\mathrm{ex}} \rangle_{cn}$ and $\langle \delta^2 N_{\mathrm{ex}} \rangle_{cn}$ are determined by two different poles, such an asymptotic difference does not exist.

Conceptually instructive as the above calculation may be, it is also lacking elegance, to say the least. The reason for the appearance of cumbersome equations like Eq. (82) or Eq. (88) lies in the fact that one exctracts the fluctuations from the exponentially large moments $\mu_k(E)$, taking the difference (55). This involves huge cancellations, as becomes dramatically clear already for $d = 1$ by comparing the numbers listed in Tables I and V of Appendix C. If one could avoid computing the microcanonical moments, and aim directly for the *difference* between canonical and microcanonical fluctuations, one should get expressions of a far simpler nature. The following section will show that such a strategy is actually feasible.

V. MELLIN-BARNES APPROACH TO MICROCANONICAL CONDENSATE FLUCTUATIONS

We start by considering the excited-states subsystem with the fugacity z and the energy E as basic variables [15], so that we have the relation $N_{\mathrm{ex}} = N_{\mathrm{ex}}(z, E)$. In principle, N_{ex} depends also on trap parameters that determine the single-particle energies, like the oscillator frequencies in the case of harmonic traps, but these parameters will be kept constant in the following. Taking the total differential,

$$\mathrm{d}N_{\mathrm{ex}} = \left(\frac{\partial N_{\mathrm{ex}}}{\partial z}\right)_E \mathrm{d}z + \left(\frac{\partial N_{\mathrm{ex}}}{\partial E}\right)_z \mathrm{d}E \,, \tag{91}$$

then keeping the temperature T fixed, one finds

$$z \left(\frac{\partial N_{\mathrm{ex}}}{\partial z}\right)_T \bigg|_{z=1} = z \left[\left(\frac{\partial N_{\mathrm{ex}}}{\partial z}\right)_E + \left(\frac{\partial N_{\mathrm{ex}}}{\partial E}\right)_z \left(\frac{\partial E}{\partial z}\right)_T\right]_{z=1} \,. \tag{92}$$

The left hand side equals the canonical mean-square fluctuation $\langle \delta^2 N_{\mathrm{ex}} \rangle_{cn}$, whereas the first term on the r.h.s. is its microcanonical counterpart $\langle \delta^2 N_{\mathrm{ex}} \rangle_{mc}$. Hence, we obtain

$$\langle \delta^2 N_{\mathrm{ex}} \rangle_{cn} - \langle \delta^2 N_{\mathrm{ex}} \rangle_{mc} = \left(\frac{\partial N_{\mathrm{ex}}}{\partial E}\right)_z \left(\frac{\partial E}{\partial z}\right)_T \bigg|_{z=1}$$
$$= \frac{k_B T^2 \left(\frac{\partial N_{\mathrm{ex}}}{\partial T}\right)_z \left(\frac{\partial E}{\partial z}\right)_T \big|_{z=1}}{k_B T^2 \left(\frac{\partial E}{\partial T}\right)_z \big|_{z=1}} \,. \tag{93}$$

Now the denominator

$$k_B T^2 \left(\frac{\partial E}{\partial T}\right)_z \bigg|_{z=1} = \langle \delta^2 E \rangle_{cn} \tag{94}$$

is the canonical mean-square fluctuation of the system's energy, whereas the two partial derivatives in the numerator,

$$k_B T^2 \left(\frac{\partial N_{\mathrm{ex}}}{\partial T}\right)_z \bigg|_{z=1} = \left(\frac{\partial E}{\partial z}\right)_T \bigg|_{z=1} = \langle \delta N_{\mathrm{ex}} \delta E \rangle_{cn} \,, \tag{95}$$

both equal the canonical particle-energy correlation $\langle \delta N_{\mathrm{ex}} \delta E \rangle_{cn} = \langle N_{\mathrm{ex}} E \rangle_{cn} - \langle N_{\mathrm{ex}} \rangle_{cn} \langle E \rangle_{cn}$. Thus, we arrive at the noteworthy identity

$$\langle \delta^2 n_0 \rangle_{cn} - \langle \delta^2 n_0 \rangle_{mc} = \frac{[\langle \delta N_{\mathrm{ex}} \delta E \rangle_{cn}]^2}{\langle \delta^2 E \rangle_{cn}} \tag{96}$$

which expresses the difference between canonical and microcanonical condensate fluctuations in terms of quantities that can be computed entirely within the convenient canonical ensemble. The usefulness of this formula, first stated by Navez et al. [15], rests in the fact that it lends itself again to the oscillator approximation, and thus to an efficient evaluation by means of the Mellin–Barnes transformation: Within the oscillator approximation, the canonical particle-energy correlation becomes

$$\langle \delta N_{\mathrm{ex}} \delta E \rangle_{cn} = \left(z \frac{\partial}{\partial z} \right) \left(-\frac{\partial}{\partial \beta} \right) \ln \Xi_{\mathrm{ex}}(z, \beta) \bigg|_{z=1}$$

$$= \sum_{\nu=1}^{\infty} \frac{\varepsilon_\nu}{\exp(\beta \varepsilon_\nu) - 1} \left(\frac{1}{\exp(\beta \varepsilon_\nu) - 1} + 1 \right)$$

$$= \frac{1}{\beta} \frac{1}{2\pi i} \int_{\tau - i\infty}^{\tau + i\infty} dt\, \Gamma(t) Z(\beta, t-1) \zeta(t-1) , \qquad (97)$$

and the canonical energy fluctuation adopts the quite similar form

$$\langle \delta^2 E \rangle_{cn} = \left(-\frac{\partial}{\partial \beta} \right)^2 \ln \Xi_{\mathrm{ex}}(z, \beta) \bigg|_{z=1}$$

$$= \sum_{\nu=1}^{\infty} \frac{\varepsilon_\nu^2}{\exp(\beta \varepsilon_\nu) - 1} \left(\frac{1}{\exp(\beta \varepsilon_\nu) - 1} + 1 \right)$$

$$= \frac{1}{\beta^2} \frac{1}{2\pi i} \int_{\tau - i\infty}^{\tau + i\infty} dt\, \Gamma(t) Z(\beta, t-2) \zeta(t-1) . \qquad (98)$$

Hence,

$$\langle \delta^2 n_0 \rangle_{cn} - \langle \delta^2 n_0 \rangle_{mc} = \frac{\left[\frac{1}{2\pi i} \int_{\tau - i\infty}^{\tau + i\infty} dt\, \Gamma(t) Z(\beta, t-1) \zeta(t-1) \right]^2}{\frac{1}{2\pi i} \int_{\tau - i\infty}^{\tau + i\infty} dt\, \Gamma(t) Z(\beta, t-2) \zeta(t-1)} . \qquad (99)$$

Compared to the saddle-point approach in the preceding section, this formula is remarkably easy to handle. Applied to the one-dimensional harmonic trap, for instance, it yields immediately

$$\langle \delta^2 n_0 \rangle_{cn} - \langle \delta^2 n_0 \rangle_{mc} = \frac{1}{2\zeta(2)} \frac{k_B T}{\hbar \omega} \left[\ln \left(\frac{k_B T}{\hbar \omega} \right) + \gamma + 1 \right]^2 . \qquad (100)$$

Improving Eq. (34) by taking also the next-to-leading pole into account,

$$\langle \delta^2 n_0 \rangle_{cn} = \zeta(2) \left(\frac{k_B T}{\hbar \omega} \right)^2 - \frac{1}{2} \frac{k_B T}{\hbar \omega} , \qquad (101)$$

and substituting $k_B T / (\hbar \omega) = \sqrt{6n}/\pi + 3/(2\pi^2)$ as stated by Eq. (67), we arrive at a refined approximation to the microcanonical ground state fluctuation:

$$\langle \delta^2 n_0 \rangle_{mc} = n - \frac{3\sqrt{6n}}{\pi^3} \left[\ln \left(\frac{\sqrt{6n}}{\pi} \right) + \gamma + 1 \right]^2 . \qquad (102)$$

As we already know, the relative difference between canonical and microcanonical mean-square fluctuations vanishes asymptotically for a condensate in a one-dimensional harmonic trap. But still, this relative difference is of the order $O(\ln^2 n / \sqrt{n})$, so that Eq. (102) is substantially more accurate than the previous leading-order approximation (74).

This fluctuation formula (102) again has an interesting number-theoretical interpretation. As indicated in the previous section, the oscillator approximation, when applied to a one-dimensional harmonic trapping potential, corresponds to neglecting the difference between

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partitions of n into no more than N summands and unrestricted partitions; this remains exact as long as $n \leq N$. Hence, Eq. (102) provides *a forteriori* a fair approximation to the fluctuation of the number of integer summands into which the integer n can be decomposed. Figure 1 depicts the r.m.s.-fluctuation $\sigma(n) = \langle \delta^2 n_0 \rangle_{mc}^{1/2}$ as approximated by Eq. (74) (upper dashed line) and by Eq. (102) (lower dashed line; coinciding almost with the full line), and compares these approximations to the exact data (full line). The latter have been computed numerically from the distribution (52) for the one-dimensional harmonic trap, utilizing the recursion relation

$$\Phi(N_{\text{ex}}|n\hbar\omega) = \sum_{k=1}^{\min(n-N_{\text{ex}},N_{\text{ex}})} \Phi(k\,|(n-N_{\text{ex}})\hbar\omega) \tag{103}$$

with $\Phi(1\,|1\,\hbar\omega) = \Phi(n|n\hbar\omega) = 1$, assuming $n \leq N$. The agreement between the exact fluctuation and the improved asymptotic formula is no less than striking. It should be noted that, within the oscillator approximation, Eq. (102) describes the fluctuation of the ground state particles not only up to the "restriction temperature" $T_R = (\hbar\omega/k_B)\sqrt{N/\zeta(2)}$, where $n = N$, but almost up to $T_0 = (\hbar\omega/k_B)N/\ln N$, where the occupation of the ground state becomes significant [10].

The handiness of the fluctuation formula (99) becomes fully clear when dealing with d-dimensional harmonic traps, $d \geq 2$. Since isotropic harmonic traps can be considered as special cases, we proceed at once to anisotropic potentials, and consider $d = 2$ first. All the required technicalities have already been collected in Section III and Appendix A: The integrand in the denominator of Eq. (99) has its rightmost pole at $t = 3$ with residue $\Gamma(3)(k_B T/\hbar\Omega)^2\zeta(2)$; the rightmost pole of the integrand in the numerator lies at $t = 4$, with residue $\Gamma(4)(k_B T/\hbar\Omega)^2\zeta(3)$. Thus,

$$\langle \delta^2 n_0 \rangle_{cn} - \langle \delta^2 n_0 \rangle_{mc} = \frac{2}{3}\frac{\zeta(2)^2}{\zeta(3)}\left(\frac{k_B T}{\hbar\Omega}\right)^2, \tag{104}$$

implying that the difference between canonical and microcanonical fluctuations is still small, even if only by a logarithm, compared to the canonical fluctuations (36) or (47), respectively. Hence, in the asymptotic limit $k_B T/(\hbar\Omega) \gg 1$ — assuming N is that large that this limit can be reached with a condensate — canonical and microcanonical condensate fluctuations still agree. But this is clearly the marginal case, as witnessed by the fact that for $d = 2$ the poles of $Z(\beta,t)$ and $\zeta(t-1)$ in Eq. (27) fall together.

For $d \geq 3$, the relevant poles in the integrands of Eq. (99) are located at $t = d+1$ and $t = d+2$, and one finds the general formula

$$\langle \delta^2 n_0 \rangle_{cn} - \langle \delta^2 n_0 \rangle_{mc} = \frac{d}{d+1}\frac{\zeta(d)^2}{\zeta(d+1)}\left(\frac{k_B T}{\hbar\Omega}\right)^d. \tag{105}$$

In particular, for isotropic three-dimensional traps one recovers, but now without any substantial effort, the previous result (90). More generally, for $d \geq 3$ the condensate fluctuations in harmonically trapped, energetically isolated ideal Bose gases are significantly smaller than the corresponding fluctuations (51) in traps that are thermally coupled to some heat bath, although the exponent of T remains the same. As we have repeatedly emphasized, this finding is explained by the fact that for $d \geq 3$ both $\langle N_{\text{ex}} \rangle_{cn}$ and $\langle \delta^2 N_{\text{ex}} \rangle_{cn}$ are determined by the same simple pole of the spectral Zeta function $Z(\beta,t)$.

VI. CONCLUSIONS

The three central formulas explained in this work, Eqs. (25), (27), and (99), vindicate the assertion put forward in the Introduction: It is the location of the rightmost pole of the spectral Zeta function $Z(\beta, t)$ that determines the statistical properties of the condensate. If that pole is located at $t = p$, and $0 < p < 1$, then we deduce from Eq. (25) that $\langle N_{\text{ex}} \rangle_{cn}$ grows linearly with temperature (so that $\langle n_0 \rangle_{cn}$ decreases linearly with T) in the condensate regime, irrespective of the detailed properties of the trap, since in that case the pole of $\zeta(t)$ lies to the right of p. If $p = 1$, the poles of $Z(\beta, t)$ and $\zeta(t)$ fall together, so that the linear temperature dependence develops a logarithmic correction. If $p > 1$, we have $\langle N_{\text{ex}} \rangle_{cn} \propto T^p$.

The key point to be noted when discussing canonical condensate fluctuations is that the pole of the Riemann Zeta function $\zeta(t-1)$ in Eq. (27) lies at $t = 2$, so that $\langle \delta^2 n_0 \rangle_{cn}$ changes its T-dependence at $p = 2$: If $0 < p < 2$, then $\langle \delta^2 n_0 \rangle_{cn} \propto T^2$; if $p = 2$, there is the familiar logarithmic correction to this quadratic T-dependence, as expressed by Eqs. (36) and (47) for two-dimensional harmonic traps; if $p > 2$, then $\langle \delta^2 n_0 \rangle_{cn} \propto T^p$.

The saddle-point calculations in Section IV may be cumbersome, but they exemplify on an elementary level why $\langle n_0 \rangle_{cn}$ equals $\langle n_0 \rangle_{mc}$ in the asymptotic regime, and why canonical and microcanonical condensate fluctuations may differ. Equation (88) summarizes the essentials for the three-dimensional oscillator trap: One needs three slightly different saddle-point parameters for computing the required microcanonical moments (53) within the oscillator approximation (12) from their canonical counterparts (11); these slight differences lower the microcanonical fluctuation against the canonical one. The elegant expression (99) links the difference $\langle \delta^2 n_0 \rangle_{cn} - \langle \delta^2 n_0 \rangle_{mc}$ again to the dominant pole of $Z(\beta, t)$: If $0 < p < 2$, that difference has an exponent of T which is smaller than that of $\langle \delta^2 n_0 \rangle_{cn}$, so that both types of fluctuations become asymptotically equal, but if $p > 2$, then the difference acquires the same exponent of T as $\langle \delta^2 n_0 \rangle_{cn}$, so that the microcanonical condensate fluctuation remains lower than the canonical one even in the asymptotic regime.

We have evaluated canonical and microcanonical condensate fluctuations explicitly for harmonic trapping potentials, where $Z(\beta, t)$ reduces to the familiar Riemann or Barnes-type Zeta functions. This may appear a bit special, but an analogous discussion is possible for quite arbitrary traps, if one merely exploits the connection between the residues of $Z(\beta, t)$ and the corresponding heat-kernel coefficients (see Ref. [36] for a brief explanation of this fairly deep connection).

The vision of letting the poles of $Z(\beta, t)$ move in the complex t-plane is not a fantasy restricted to the theorist's ivory tower, but may have direct experimental consequences. Continuously deforming the trapping potential means continuously changing the trap's single-particle spectrum, and hence shifting p. For example, a spectrum of the type [22,14]

$$\varepsilon_{\nu_1, \ldots, \nu_d} = \varepsilon_0 \sum_{i=1}^{d} c_i \nu_i^s \tag{106}$$

with integer quantum numbers ν_i and dimensionless anisotropy coefficients c_i not too different from unity implies $p = d/s$ [16], so that, e.g., steepening a three-dimensional harmonic oscillator potential ($s = 1$) towards a box potential ($s = 2$) means lowering p from 3 to 3/2. During such a process, the fluctuation of a large condensate is described by an exponent

of T that *changes* as long as p remains above 2, since then $\langle \delta^2 n_0 \rangle_{mc} \propto T^{d/s}$, but *remains constant* when p decreases further; $\langle \delta^2 n_0 \rangle_{mc} \propto T^2$.

There is another detail that deserves to be mentioned. From the viewpoint of partition theory, Eq. (74) states that the r.m.s.-fluctuation of the number of parts into which a large integer n can be decomposed is approximately normal, $\sigma(n) \sim \sqrt{n}$. However, when characterizing condensate fluctuations, one would not do so in terms of the number of excitation quanta n, but rather in terms of the number of excited particles $\langle N_{\mathrm{ex}} \rangle_{mc}$ [3]. But then Eqs. (71) and (74) yield

$$\langle \delta^2 N_{\mathrm{ex}} \rangle_{mc}^{1/2} \; \propto \; \langle N_{\mathrm{ex}} \rangle_{mc} \, , \tag{107}$$

apart from logarithmic corrections, stating that the *normal* partition-theoretic fluctuation translates into *supranormal* fluctuation of the number of excited Bose particles in a one-dimensional harmonic trap. More generally, for traps with single-particle spectra (106) one obtains [16]

$$
\begin{aligned}
\langle \delta^2 N_{\mathrm{ex}} \rangle^{1/2} &\propto \langle N_{\mathrm{ex}} \rangle & \text{for} \quad & 0 < d/s < 1 \, , \\
\langle \delta^2 N_{\mathrm{ex}} \rangle^{1/2} &\propto \langle N_{\mathrm{ex}} \rangle^{s/d} & \text{for} \quad & 1 < d/s < 2 \, , \\
\langle \delta^2 N_{\mathrm{ex}} \rangle^{1/2} &\propto \langle N_{\mathrm{ex}} \rangle^{1/2} & \text{for} \quad & 2 < d/s \, ;
\end{aligned}
\tag{108}
$$

both within the canonical and the microcanonical ensemble. Hence, when increasing d/s from the $1d$-harmonic oscillator value 1, the degree of supranormality is gradually lowered, until one arrives at normal particle number fluctuations for $d/s > 2$.

Taking these insights together with those obtained in the related previous works [10–16], it seems fair to conclude that by now a classic problem in statistical mechanics, the fluctuation of an ideal Bose–Einstein condensate, has been fully understood.

APPENDIX A: RESIDUES OF BARNES-TYPE ZETA FUNCTIONS

According to Section III, the spectral Zeta function for d-dimensional anisotropic harmonic traps adopts the Barnes form

$$Z(\beta, t) \; = \; \sum_{\vec{\nu} \in \mathbb{N}_0^d / \{0\}} \frac{1}{(\beta \hbar \vec{\omega} \vec{\nu})^t} \, , \tag{A1}$$

and the canonical thermodynamics of an ideal Bose gas stored in such a trap depends crucially on the rightmost pole of this function. In this appendix we briefly sketch the derivation of Eq. (44), i.e., of the residue of the rightmost pole of $Z(\beta, t)$.

The starting point is the contour integral representation of the Gamma function [37],

---

[3] We choose to characterize the fluctuation in terms of $\langle N_{\mathrm{ex}} \rangle$, rather than $\langle n_0 \rangle$, since the properties of an ideal Bose–Einstein condensate, including its fluctuation, are independent of $\langle n_0 \rangle$. This is just what is exploited in the oscillator approximation.

$$\Gamma(t) = \frac{i}{2\sin(\pi t)} \int_{\mathcal{C}} d\alpha \, (-\alpha)^{t-1} e^{-\alpha} , \tag{A2}$$

where $\mathcal{C}$ is enclosing the positive real axis counterclockwise. With the help of this representation we deduce

$$\begin{aligned} Z(\beta,t) &= \frac{i}{2\sin(\pi t)\,\Gamma(t)} \int_{\mathcal{C}} d\alpha \, (-\alpha)^{t-1} e^{-\alpha} \sum_{\vec{\nu}\in\mathbb{N}_0^d/\{0\}} \frac{1}{(\beta\hbar\vec{\omega}\vec{\nu})^t} \\ &= \frac{i}{2\sin(\pi t)\,\Gamma(t)} \sum_{\vec{\nu}\in\mathbb{N}_0^d/\{0\}} \int_{\mathcal{C}} d\alpha \, (-\alpha)^{t-1} e^{-\alpha\beta\hbar\vec{\omega}\vec{\nu}} \\ &= -\frac{\Gamma(1-t)}{2\pi i} \int_{\mathcal{C}} d\alpha \, (-\alpha)^{t-1} \left\{ \frac{1}{\prod_{i=1}^{d}(1-e^{-\alpha\beta\hbar\omega_i})} - 1 \right\} . \end{aligned} \tag{A3}$$

The first equality is obtained by interchanging summation and integration, then changing in each summand from the integration variable α to $\alpha\beta\hbar\vec{\omega}\vec{\nu}$; the second by summing the resulting geometric series and utilizing the relation

$$\sin(\pi t)\,\Gamma(t) = \frac{\pi}{\Gamma(1-t)} . \tag{A4}$$

The poles of $Z(\beta,t)$ are featured by Eq. (A3) in a particularly transparent manner. Namely, the prefactor $\Gamma(1-t)$ has simple poles at integer values $t = 1, 2, 3, \ldots$. At these values the remaining contour integral may be evaluated immediately by just collecting the residues enclosed by $\mathcal{C}$. The only possible pole contributing to the integral lies at $\alpha = 0$; it has nonvanishing residues for $t = -\infty, \ldots, -1, 0, 1, \ldots, d$. Hence, the poles of $Z(\beta,t)$ are located at $t = 1, \ldots, d$, and the residue of the rightmost pole is found to be

$$\operatorname{res} Z(\beta,d) = (-1)^{d-1} \prod_{i=1}^{d} (\beta\hbar\omega_i)^{-1} \operatorname{res} \Gamma(1-d) . \tag{A5}$$

Using the identity

$$\operatorname{res} \Gamma(-n) = \frac{(-1)^n}{n!} , \qquad n \in \mathbb{N}_0 , \tag{A6}$$

we arrive directly at Eq. (44).

APPENDIX B: CANONICAL CONDENSATE FLUCTUATION FOR $D = 2$

When evaluating the fluctuation formula (27) for two-dimensional harmonic traps, the product $Z(\beta,t)\,\zeta(t-1)$ provides a double pole at $t = 2$. In that case the knowledge of the residue (44) is not enough for computing the mean-square condensate fluctuation; also the finite part of $Z(\beta,t)$ at $t = 2$ enters into the residue of the double pole. More precisely, in analogy to Eq. (31) for the Riemann Zeta function, one needs the expansion

$$Z(\beta,t) = \left(\frac{k_B T}{\hbar\Omega}\right)^2 \left(\frac{1}{t-2} + f(\omega_1,\omega_2,t)\right) \tag{B1}$$

for t close to 2. In this appendix we determine the function $f(\omega_1, \omega_2, t)$, and thus prove Eq. (47).

Introducing $a = \sqrt{\omega_1/\omega_2}$ and $b = \sqrt{\omega_2/\omega_1}$, we first write

$$Z(\beta, t) = \left(\frac{k_B T}{\hbar\Omega}\right)^t \sum_{\vec{\nu} \in \mathbb{N}_0^2/\{0\}} \frac{1}{(a\nu_1 + b\nu_2)^t} , \tag{B2}$$

valid for $\mathcal{R}e\,(t) > 2$. Splitting the sum according to the scheme

$$\sum_{\vec{\nu} \in \mathbb{N}_0^2/\{0\}} = \sum_{\nu_1=1}^{\infty} (\nu_2 = 0) + \sum_{\nu_2=1}^{\infty} (\nu_1 = 0) + \sum_{\nu_1,\nu_2=1}^{\infty} ,$$

we find the decomposition

$$Z(\beta, t) = \left(\frac{k_B T}{\hbar\Omega}\right)^t \left\{ \zeta(t)(a^{-t} + b^{-t}) + H(\omega_1, \omega_2, t) \right\} , \tag{B3}$$

where

$$H(\omega_1, \omega_2, t) = \sum_{\nu_1,\nu_2=1}^{\infty} \frac{1}{(a\nu_1 + b\nu_2)^t}$$

$$= \frac{1}{\Gamma(t)} \int_0^\infty d\alpha\, \alpha^{t-1} \frac{e^{-(a+b)\alpha}}{(1 - e^{-a\alpha})(1 - e^{-b\alpha})} . \tag{B4}$$

This identity is obtained in a similar manner as Eq. (A3), using the familiar representation

$$\Gamma(t) = \int_0^\infty d\alpha\, \alpha^{t-1} e^{-\alpha} \tag{B5}$$

of the Gamma function.

Now we are interested in the behaviour of $Z(\beta, t)$ as $t \to 2$, where, as we know from Appendix A, it has a simple pole. How is this realized in Eq. (B3)? Since $\zeta(t)$ is regular at $t = 2$, the pole is contained in the integral (B4). At the lower integration bound, that is, for $\alpha \to 0$, the integrand behaves as $1/\alpha$ for $t \to 2$; therefore the integral diverges at $t = 2$. The behaviour of the integral as t tends to 2 is extracted with the help of the following trick. For $\mathcal{R}e\,(t) > 2$, write

$$H(\omega_1, \omega_2, t) = \frac{1}{\Gamma(t)} \int_0^\infty d\alpha\, \alpha^{t-1} e^{-(a+b)\alpha} \left(\frac{1}{(1 - e^{-a\alpha})(1 - e^{-b\alpha})} - \frac{1}{\alpha^2} + \frac{1}{\alpha^2} \right)$$

$$= \frac{\Gamma(t-2)}{\Gamma(t)} (a+b)^{2-t}$$

$$+ \frac{1}{\Gamma(t)} \int_0^\infty d\alpha\, \alpha^{t-1} e^{-(a+b)\alpha} \left(\frac{1}{(1 - e^{-a\alpha})(1 - e^{-b\alpha})} - \frac{1}{\alpha^2} \right) ,$$

where Eq. (B5) has been used. The simple pole of $Z(\beta, t)$ at $t = 2$ is now contained in the first term, since $\Gamma(t-2)/\Gamma(t) = 1/[(t-1)(t-2)]$, and the remaining integral is finite for $t = 2$. In this way, we arrive at the expansion

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$$H(\omega_1, \omega_2, t) = \frac{1}{t-2} - 1 - \ln\left(\sqrt{\frac{\omega_1}{\omega_2}} + \sqrt{\frac{\omega_2}{\omega_1}}\right) + I(\omega_1, \omega_2) + O(t-2) , \qquad \text{(B6)}$$

with $I(\omega_1, \omega_2)$ as defined in Eq. (48). Together with Eq. (B3), this determines the desired function $f(\omega_1, \omega_2, t)$ and thereby leads to the result (47).

It is quite interesting to see how the fluctuation formula (36) for the isotropic case is recovered in the limit $\omega_1 = \omega_2 = \omega$. Then the integral simplifies to

$$
\begin{aligned}
I(\omega, \omega) &= \int_0^\infty d\alpha\, \alpha e^{-2\alpha} \left(\frac{1}{(1-e^{-\alpha})^2} - \frac{1}{\alpha^2}\right) \\
&= 2 - \int_0^\infty d\alpha \left[e^{-2\alpha}\left(\frac{1}{\alpha} - \frac{1}{1-e^{-\alpha}}\right) + \frac{\alpha e^{-\alpha}}{1-e^{-\alpha}} \right] .
\end{aligned}
\qquad \text{(B7)}
$$

Employing now the identities [37]

$$\psi(z) = \frac{d}{dz} \ln \Gamma(z) = \ln z + \int_0^\infty d\alpha\, e^{-z\alpha}\left(\frac{1}{\alpha} - \frac{1}{1-e^{-\alpha}}\right) \qquad \text{(B8)}$$

for the Psi function, and

$$\zeta_H(z, q) = \sum_{n=0}^\infty \frac{1}{(n+q)^z} = \frac{1}{\Gamma(z)} \int_0^\infty d\alpha\, \frac{\alpha^{z-1} e^{-q\alpha}}{1-e^{-\alpha}} \qquad \text{(B9)}$$

for the Hurwitz Zeta function, we end up with Eq. (49). This equation confirms that the complicated expression (47) for the canonical condensate fluctuation in a two-dimensional anisotropic harmonic trap indeed becomes equal to the expression (36) in the isotropic limit.

APPENDIX C: MOMENTS OF PARTITIONS

The saddle-point method followed in Section IV can be employed to derive asymptotic expressions for the k-th moments $\mu_k(n)$ of unrestricted partitions of integer n, for arbitrary k [19]. Defining the symbol

$$\sum [\lambda_0, \lambda_1, \ldots, \lambda_{k-1}] \equiv \sum \frac{k!}{\ell_1! \, \ell_2! \, \ldots \, \ell_k!} \left(\frac{\lambda_0}{1!}\right)^{\ell_1} \cdots \left(\frac{\lambda_{k-1}}{k!}\right)^{\ell_k} , \qquad \text{(C1)}$$

where the sum extends over all partitions of k, i.e., $\ell_1 + 2\ell_2 + \ldots + k\ell_k = k$, we find

$$\mu_k(n) \sim \frac{1}{4\sqrt{3}n} \exp\left(\pi\sqrt{\frac{2n}{3}}\right) \left(\frac{\sqrt{6n}}{\pi}\right)^k \sum \left[\ln\left(\frac{\sqrt{6n}}{\pi}\right) + \gamma, \zeta(2), 2!\,\zeta(3), \ldots, (k-1)!\,\zeta(k)\right] .$$

$$\text{(C2)}$$

For $k = 0$, this expression gives the Hardy–Ramanujan formula (75); for $k = 1$, 2, and 3, it adopts the forms

$$\mu_1(n) \sim \mu_0(n) \frac{\sqrt{6n}}{\pi} \left[\ln\left(\frac{\sqrt{6n}}{\pi}\right) + \gamma \right] , \tag{C3}$$

$$\mu_2(n) \sim \mu_0(n) \left(\frac{\sqrt{6n}}{\pi}\right)^2 \left[\left(\ln\left(\frac{\sqrt{6n}}{\pi}\right) + \gamma\right)^2 + \zeta(2) \right] , \tag{C4}$$

$$\mu_3(n) \sim \mu_0(n) \left(\frac{\sqrt{6n}}{\pi}\right)^3 \left[\left(\ln\left(\frac{\sqrt{6n}}{\pi}\right) + \gamma\right)^3 + 3\left(\ln\left(\frac{\sqrt{6n}}{\pi}\right) + \gamma\right)\zeta(2) + 2\zeta(3) \right] . \tag{C5}$$

Note that our result (C2) differs for $k \geq 2$ from the formula stated by Richmond [19], and remedies the discrepancies found by this author when comparing his formula with exact numerical data. In fact, the above expressions are fairly accurate; some exact values of $\mu_k(n)$ for $k = 0$ to 3 are iuxtaposed in Tables I to IV to the respective asymptotic predictions. For completeness, exact values of the r.m.s.-fluctuation $\sigma(n)$ of the number of parts occuring in unrestricted partitions of n are listed in Table V, together with the approximation furnished by Eq. (102). Comparing the numbers in this table to those in Table I, one gets a vivid impression what it means to isolate microcanonical fluctuations from an exponentially large background.

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FIGURES

FIG. 1. R.m.s.-fluctuation $\sigma(n)$ of the number of integer summands into which the integer n can be partitioned. The upper dashed line is the leading approximation $\sigma(n) \sim \sqrt{n}$; the lower dashed line (coinciding almost with the full line) is the more accurate approximation obtained from the square root of Eq. (102). The full line indicates the exact values. Some numerical data are listed in Table V of Appendix C. From the viewpoint of statistical mechanics, the upper dashed line gives the r.m.s.-fluctuation of the number of ground state particles for an ideal Bose gas in a one-dimensional harmonic oscillator trap kept in contact with some heat bath, such that the average number n of excitation quanta does not exceed the particle number. The other two lines correspond to the (approximate and exact) microcanonical condensate fluctuation, that is, to the r.m.s.-fluctuation of the number of ground state particles when the gas is totally isolated from its surrounding, carrying n excitation quanta.

TABLES

n	$\mu_0(n)$ (exact)	$\mu_0(n)$ (asymptotic)	rel. error
50	$0.2042260 \cdot 10^6$	$0.2175905 \cdot 10^6$	0.0654
100	$0.1905693 \cdot 10^9$	$0.1992809 \cdot 10^9$	0.0457
200	$0.3972999 \cdot 10^{13}$	$0.4100251 \cdot 10^{13}$	0.0320
300	$0.9253083 \cdot 10^{16}$	$0.9494095 \cdot 10^{16}$	0.0260
500	$0.2300165 \cdot 10^{22}$	$0.2346387 \cdot 10^{22}$	0.0201
1000	$0.2406147 \cdot 10^{32}$	$0.2440200 \cdot 10^{32}$	0.0142
1500	$0.1329462 \cdot 10^{40}$	$0.1344797 \cdot 10^{40}$	0.0115

TABLE I. Comparison of exact numbers $\mu_0(n)$ of unrestricted partitions of n with the Hardy–Ramanujan approximation (75).

n	$\mu_1(n)$ (exact)	$\mu_1(n)$ (asymptotic)	rel. error
50	$0.2805218 \cdot 10^7$	$0.2740428 \cdot 10^7$	0.0231
100	$0.4144913 \cdot 10^{10}$	$0.4087936 \cdot 10^{10}$	0.0137
200	$0.1357412 \cdot 10^{15}$	$0.1346191 \cdot 10^{15}$	0.0083
300	$0.4102848 \cdot 10^{18}$	$0.4077577 \cdot 10^{18}$	0.0062
500	$0.1411488 \cdot 10^{24}$	$0.1405470 \cdot 10^{24}$	0.0043
1000	$0.2281551 \cdot 10^{34}$	$0.2275624 \cdot 10^{34}$	0.0026
1500	$0.1621438 \cdot 10^{42}$	$0.1618281 \cdot 10^{42}$	0.0019

TABLE II. Comparison of exact first moments $\mu_1(n)$ of unrestricted partitions of n with the asymptotic formula (C3).

n	$\mu_2(n)$ (exact)	$\mu_2(n)$ (asymptotic)	rel. error
50	$0.4461898 \cdot 10^8$	$0.4539366 \cdot 10^8$	0.0174
100	$0.1027721 \cdot 10^{12}$	$0.1037857 \cdot 10^{12}$	0.0099
200	$0.5209742 \cdot 10^{16}$	$0.5239850 \cdot 10^{16}$	0.0058
300	$0.2027390 \cdot 10^{20}$	$0.2036083 \cdot 10^{20}$	0.0043
500	$0.9563321 \cdot 10^{25}$	$0.9591871 \cdot 10^{25}$	0.0030
1000	$0.2361756 \cdot 10^{36}$	$0.2366168 \cdot 10^{36}$	0.0019
1500	$0.2146020 \cdot 10^{44}$	$0.2149100 \cdot 10^{44}$	0.0014

TABLE III. Comparison of exact second moments $\mu_2(n)$ of unrestricted partitions of n with the asymptotic formula (C4).

n	$\mu_3(n)$ (exact)	$\mu_3(n)$ (asymptotic)	rel. error
50	$0.8145597 \cdot 10^9$	$0.9334154 \cdot 10^9$	0.1459
100	$0.2898292 \cdot 10^{13}$	$0.3173679 \cdot 10^{13}$	0.0950
200	$0.2249985 \cdot 10^{18}$	$0.2390975 \cdot 10^{18}$	0.0627
300	$0.1120055 \cdot 10^{22}$	$0.1175340 \cdot 10^{22}$	0.0494
500	$0.7186145 \cdot 10^{27}$	$0.7449881 \cdot 10^{27}$	0.0367
1000	$0.2683336 \cdot 10^{38}$	$0.2749645 \cdot 10^{38}$	0.0247
1500	$0.3099702 \cdot 10^{46}$	$0.3160662 \cdot 10^{46}$	0.0197

TABLE IV. Comparison of exact third moments $\mu_3(n)$ of unrestricted partitions of n with the asymptotic formula (C5).

n	$\sigma(n)$ (exact)	$\sigma(n)$ (asymptotic)	rel. error
50	5.46	5.65	0.0349
100	8.14	8.29	0.0190
200	12.00	12.12	0.0104
300	15.00	15.11	0.0073
500	19.80	19.89	0.0047
1000	28.71	28.79	0.0026
1500	35.60	35.66	0.0018

TABLE V. Comparison of exact r.m.s.-fluctuations $\sigma(n)$ of the number of parts in unrestricted partitions of n with the predictions obtained by taking the square root of the asymptotic Eq. (102).